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Title: Exploring the Role of Viscosity in Inertial Confinement Fusion Implosions

Author(s): Dumitru, Ioana Diana
Angermeier, William
Scheiner, Brett Stanford
Sauppe, Joshua Paul

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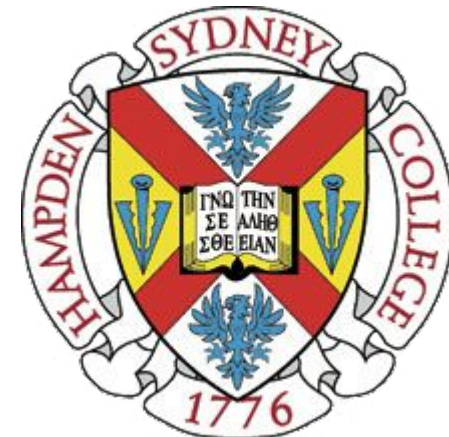
Exploring the Role of Viscosity in Inertial Confinement Fusion Implosions

Students: Alex Angermeier and Ioana Dumitru
Mentors: Brett Scheiner and Joshua Sauppe

XCP Computational Physics Student Summer Workshop
Final Presentations
August 10-12, 2021

Alex Angermeier

- Education
 - B.S. in Physics and Applied Mathematics
 - Pursuing PhD in Physics
- Research Interests
 - Computational simulations of warm dense matter
 - Development of wave packet molecular dynamics methods
 - Z-pinch and other pulsed power experiments
- Personal Interests
 - Bladesmithing
 - learning Punjabi



Ioana Dumitru

Education

- B.S in Mechanical Engineering

Research Interest include:

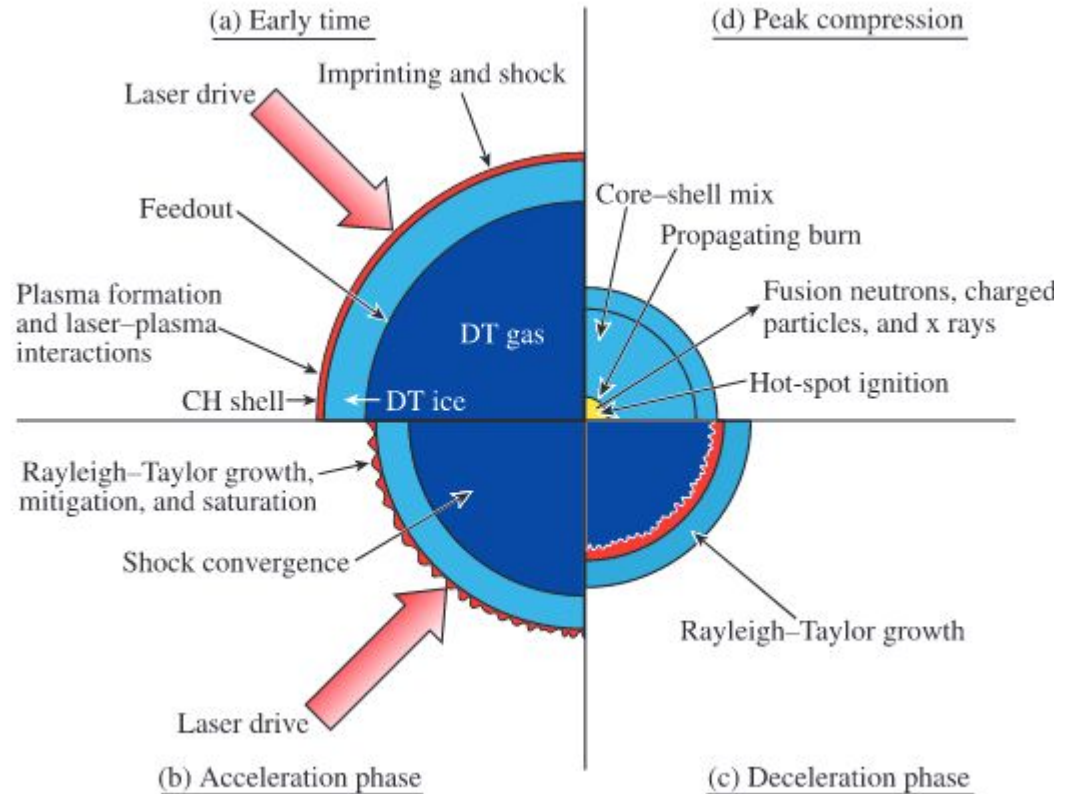
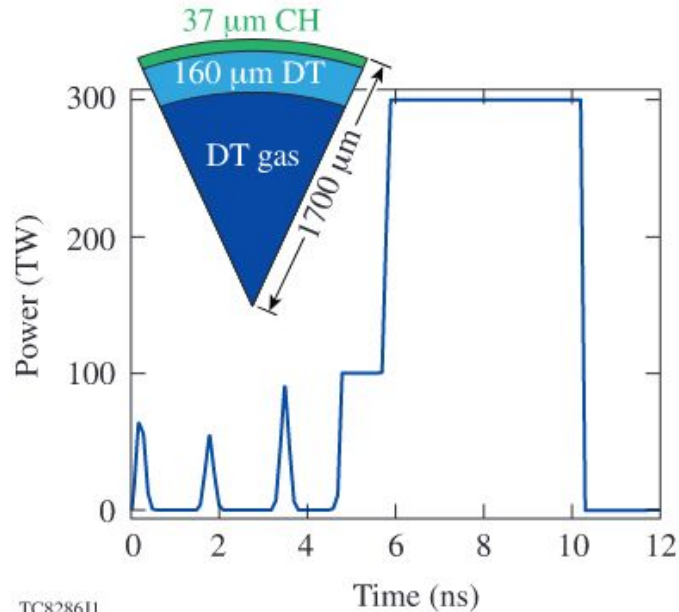
- Using simulations to understand events that impact the environment (energy/water systems, wildfires, etc.)
- Inverse Modeling

Personal Interests

- Tropical plants
- Working on cars
- Camping



General Inertial Confinement Fusion (ICF) Implosions

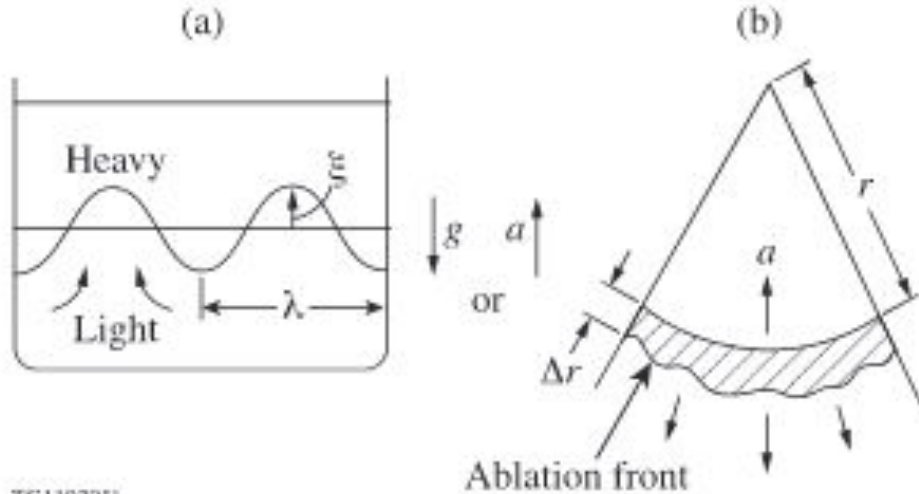


S. Craxton et al. Physics of Plasmas 22, 110501 (2015)

Hydrodynamic Instabilities

Rayleigh-Taylor

$$a_k(t) = a_k(0)e^{-\gamma(k)t}$$

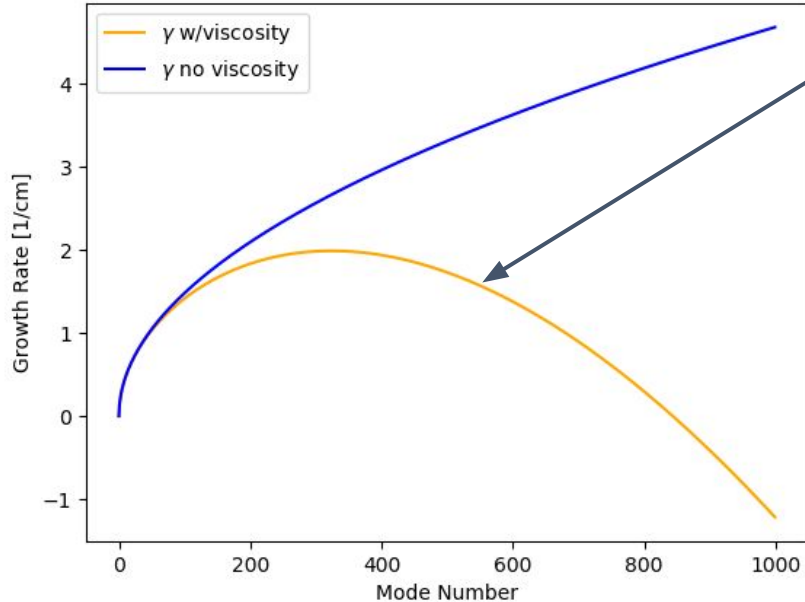


TC11929/J1

S. Craxton et al. Physics of Plasmas 22, 110501 (2015)



Hydrodynamic Instabilities are Stabilized using Viscosity



Plot showing how viscosity dampens the growth rate.

Viscous Stabilization



Viscosity represents the internal resistance of a fluid to motion.

Two-Pronged Approach to Understand Viscosity in Plasmas

Alex: micro scale approach

Molecular Dynamics Simulation (LAMMPS):

- Develop and validate a two component plasma input deck.
- Calculate the viscosity for CH mixtures at different thermodynamic conditions.

Ioana: macro scale approach

Radiation Hydrodynamics Simulation (xRage):

- Fuel target design
- Empirical calculations of viscosity
- Large sweep of physical parameter space for ICF Implosion.

Methods and Results - Molecular Dynamics (MD) with LAMMPS

One Component Plasma (OCP)

OCP: Electrons are treated as a uniform neutralizing, non-polarizable background, and there is one mobile ion species.

- Ions interact through the Coulomb potential.
- Characterized through Coulomb coupling parameter:

$$\Gamma = \frac{\langle \text{Potential Energy} \rangle}{\langle \text{Kinetic Energy} \rangle}$$

- $\Gamma > 1$: plasma is strongly coupled
- $\Gamma < 1$: plasma is weakly coupled (classical plasma physics regime)

Two Component Plasma (TCP)

TCP: Similar to OCP, except there are two mobile ions in the plasma.

- Average values for the two ion species: $\langle P \rangle = x_1 P_1 + x_2 P_2$, P represents a physical ion quantity [1].
 - n_i = number density of ion species i
 - $x_i = n_i/n$ = mole fraction of ion species i
- Treat TCP in a similar manner as the OCP
 - Single coupling parameter, plasma frequency, ion sphere radius

$$\bar{\Gamma} = x_1 \Gamma_1 + x_2 \Gamma_2 = \left\langle Z^{\frac{5}{3}} \right\rangle \langle Z \rangle^{\frac{1}{3}} \Gamma_0 \quad \text{➤ Estimated Coulomb coupling for TCP [1]}$$

$$\omega_p = \sqrt{\frac{n \langle Z \rangle^2 e^2}{\epsilon_0 \langle m \rangle}} \quad \text{➤ Aggregate plasma frequency [1]}$$

- Γ_0 = OCP Coulomb coupling parameter
- $\langle Z \rangle$ = average charge state of the TCP
- a = mean ion sphere radius
- $\langle m \rangle$ = average mass of the TCP

Transport coefficients and Green-Kubo (GK) relation

- Relates thermodynamic fluxes and forces
 - flux (transport phenomena) = rate of flow of a property (i.e. mass, energy, momentum) per unit area [1]
 - Viscosity (η) relates the momentum flux to the velocity gradient.
- GK relations connect equilibrium fluctuations of fluxes to transport coefficients[2].

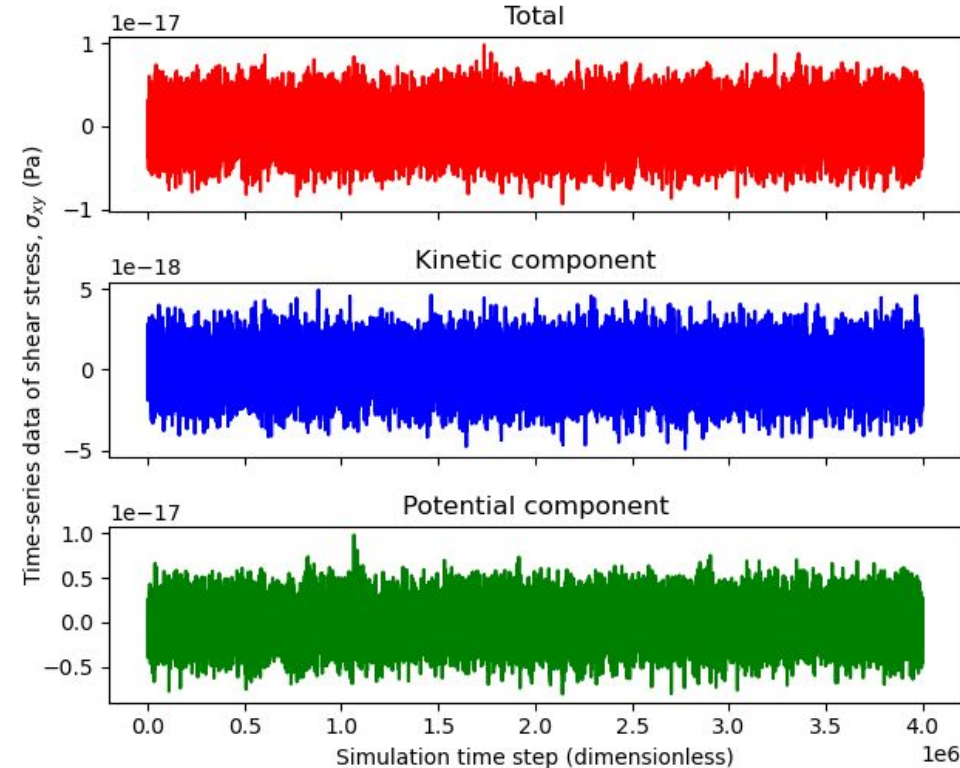
Shear viscosity [2,3]:
$$\eta = \frac{1}{Vk_B T} \int_0^\infty \langle \sigma_{xy}(t) \sigma_{xy}(0) \rangle_{eq} dt$$

- $\langle \sigma_{xy}(t) \sigma_{xy}(0) \rangle_{eq}$ = shear stress autocorrelation function
- V is the volume of the system

Molecular Dynamics Methods

Using MD to extract viscosity

TCP H-C Mix: $\bar{\Gamma} = 24.555654554$



- Equilibrate TCP system.
- Run the TCP simulation.
- Output shear stress ($\sigma_{\alpha\beta}$) in time intervals.

$$\sigma_{\alpha\beta} = \sigma_{\alpha\beta}^{kin} + \sigma_{\alpha\beta}^{pot}$$

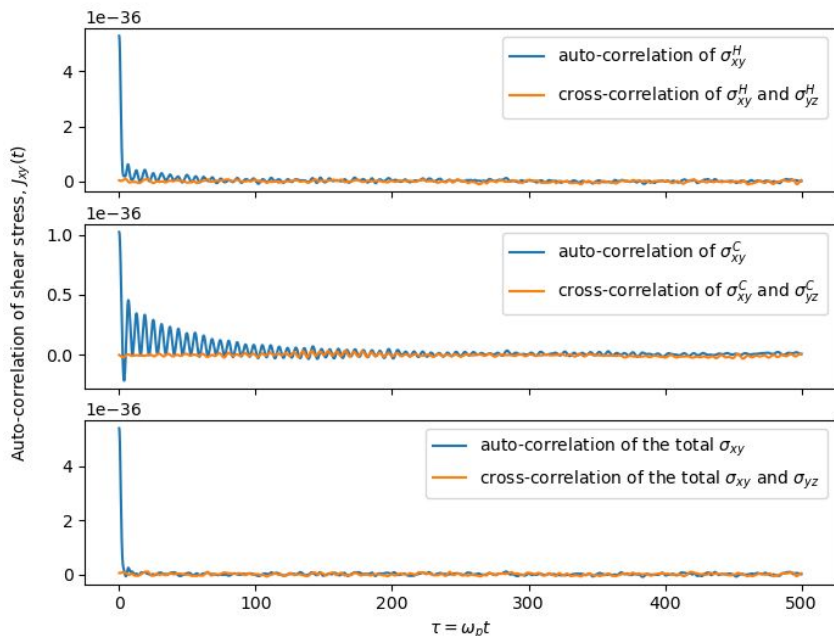
$$\sigma_{\alpha\beta}^{kin} = \frac{1}{V} \sum_{i=1}^N m(\mathbf{v}_i \cdot \hat{\alpha})(\mathbf{v}_i \cdot \hat{\beta})$$

$$\sigma_{\alpha\beta}^{pot} = \frac{1}{2V} \sum_{i=1}^N \sum_{i \neq j}^N \frac{(\mathbf{r}_{ij} \cdot \hat{\alpha})(\mathbf{r}_{ij} \cdot \hat{\beta})\phi'(r_{ij})}{r_{ij}}$$

Using MD to extract viscosity

Plot of Autocorrelation

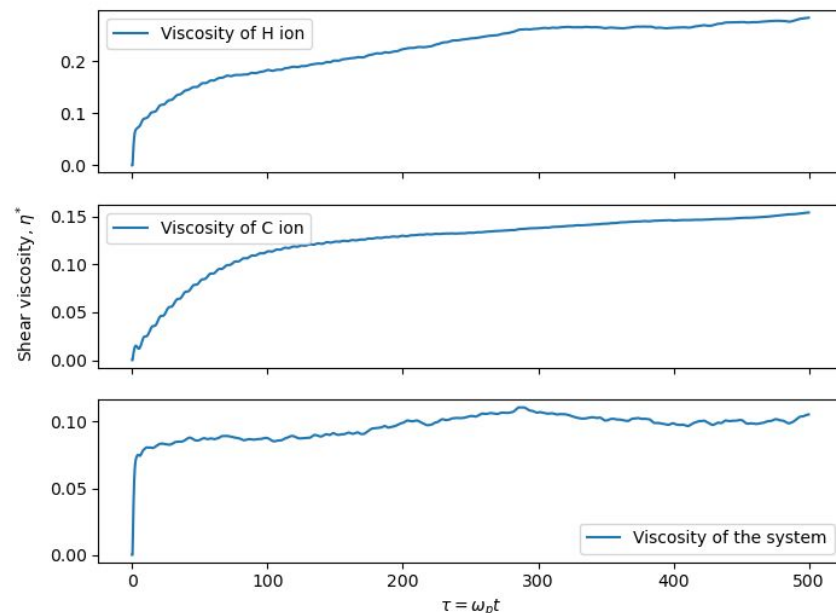
TCP H-C Mix: $\bar{\Gamma} = 24.555654554$



$$\langle \sigma_{xy}(t) \sigma_{xy}(0) \rangle_{eq}$$

Plot of Cumulative Integral

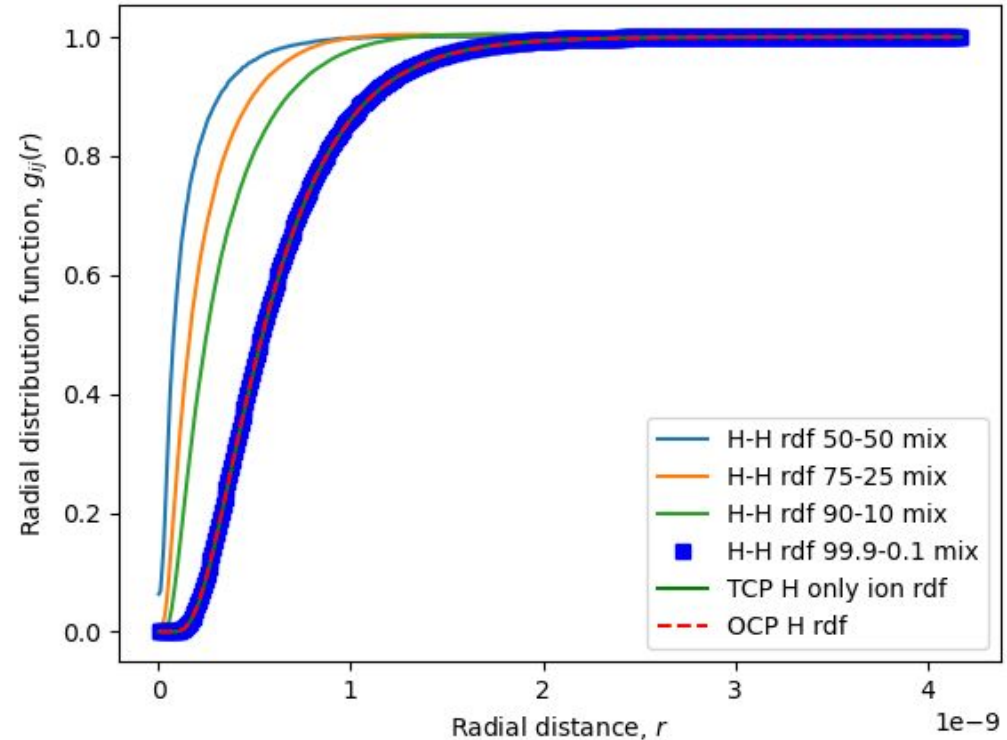
TCP H-C Mix: $\bar{\Gamma} = 24.555654554$



$$\eta = \frac{1}{Vk_B T} \int_0^\infty \langle \sigma_{xy}(t) \sigma_{xy}(0) \rangle_{eq} dt$$

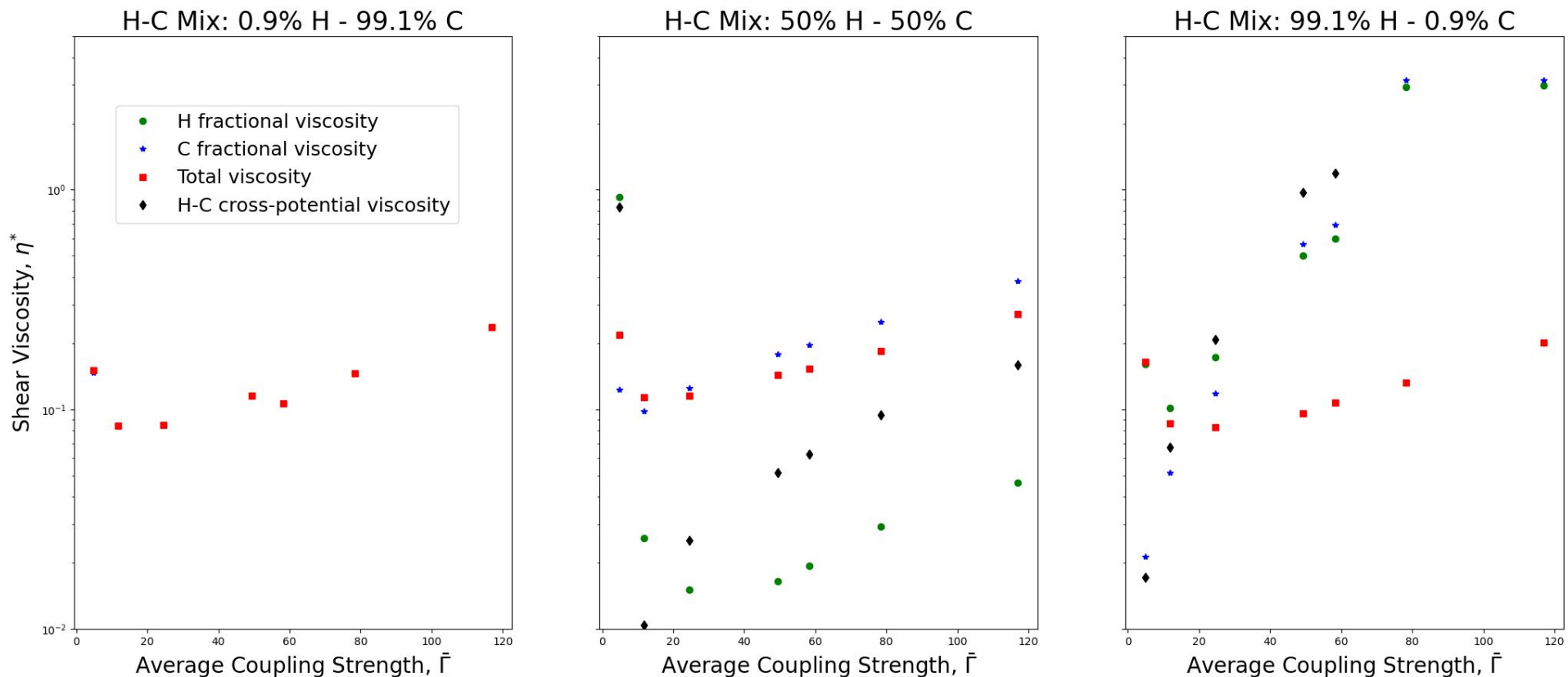
LAMMPS TCP input deck verification and validation

- Compare with well developed OCP deck
 - use the same ion for both ions in TCP deck
 - Compare equilibrium thermodynamics
 - Compare radial distribution functions (rdf)
- Use the impurity limit
 - limit the amount of one type of species to zero and compare with OCP
- Test for simulation convergence.



Molecular Dynamics Results

Results



◆ cross-potential viscosity shown is the absolute value as the cross-potential viscosity is actually negative

Methods and Results - Radiation Hydrodynamics with xRAGE

Characterizing ICF Implosions

Choose Inputs:

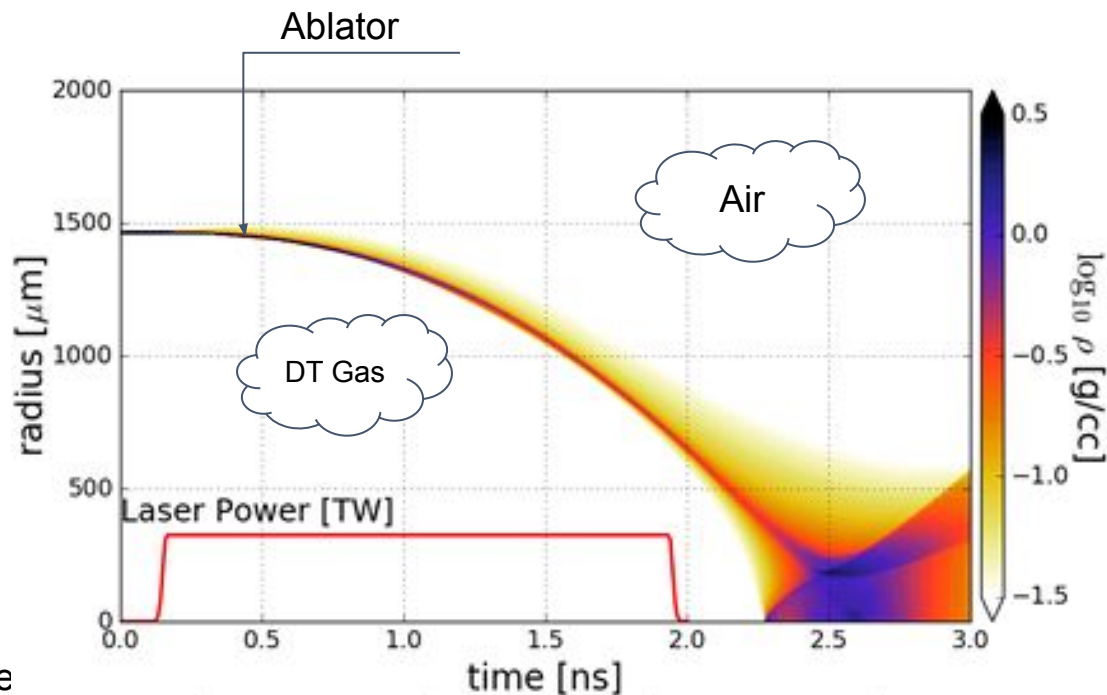
- Laser Inputs:
 - Laser pulse shapes
- Target Design
 - Carbon
 - Beryllium
 - Aluminum
 - Chromium

Note: All ablators were mass matched.

Run Model:

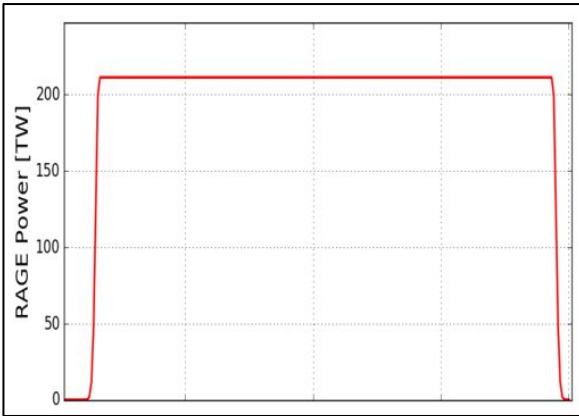
xRAGE:

- An Eulerian radiation-hydrodynamics code with adaptive mesh refinement (AMR).

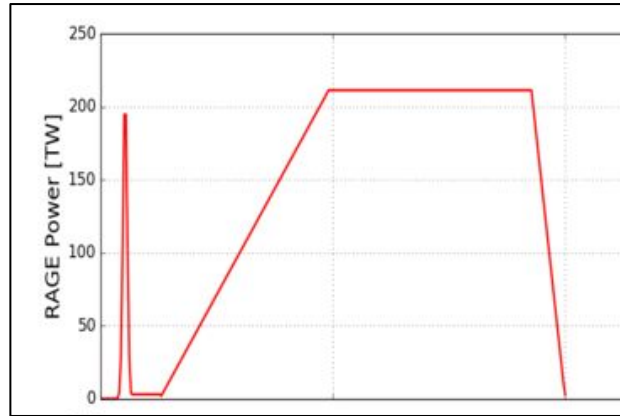


Laser Shapes Used

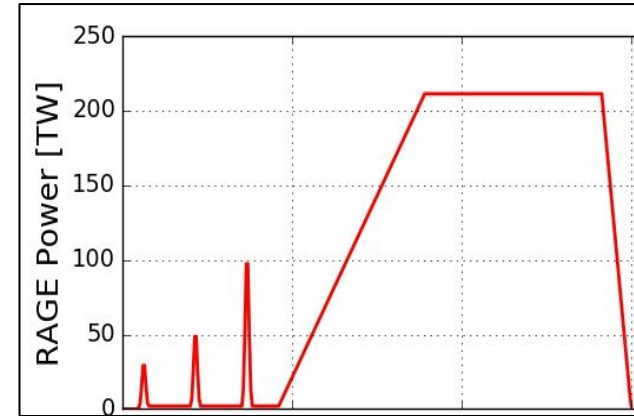
Square Wave



1-Picket



3-Picket



- Total energy for all laser shapes are the same
- Will continue discussion with square wave laser due to small variation in results.

Two Viscosity Models for Different Plasma Regimes

Viscosity for $\Gamma > 10$:

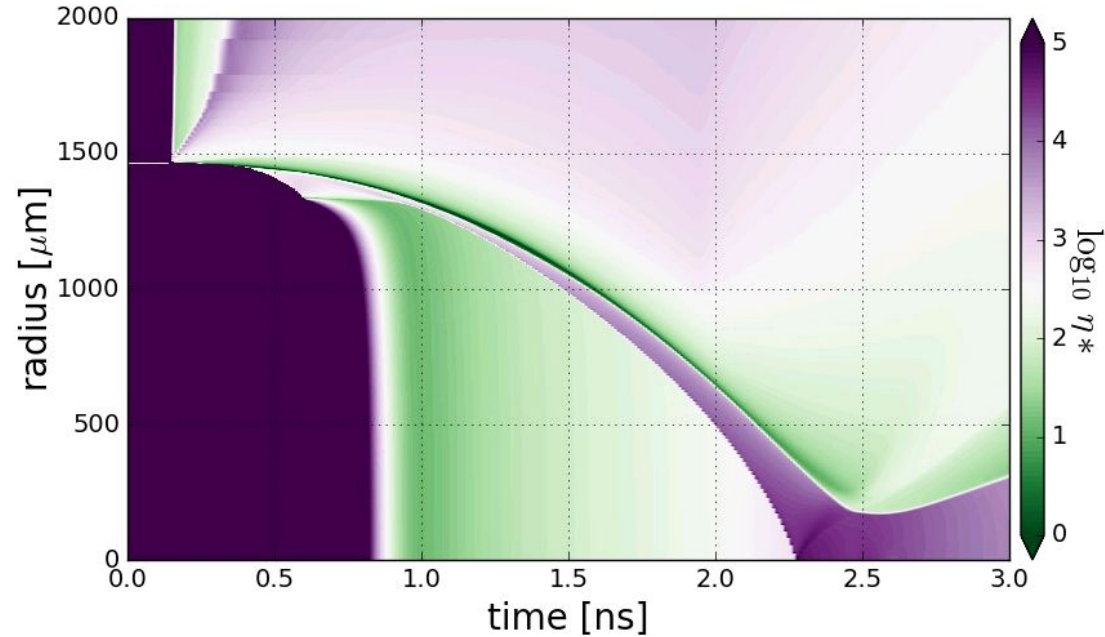
$$\eta_{\text{YVM}}^*(\kappa, \Gamma) = 0.0051 \frac{\Gamma_m}{\Gamma} + 0.374 \frac{\Gamma}{\Gamma_m} + 0.022$$

S. Bergeson et al. Physics of Plasmas 26 100501 (2019)

Viscosity for $\Gamma < 10$:

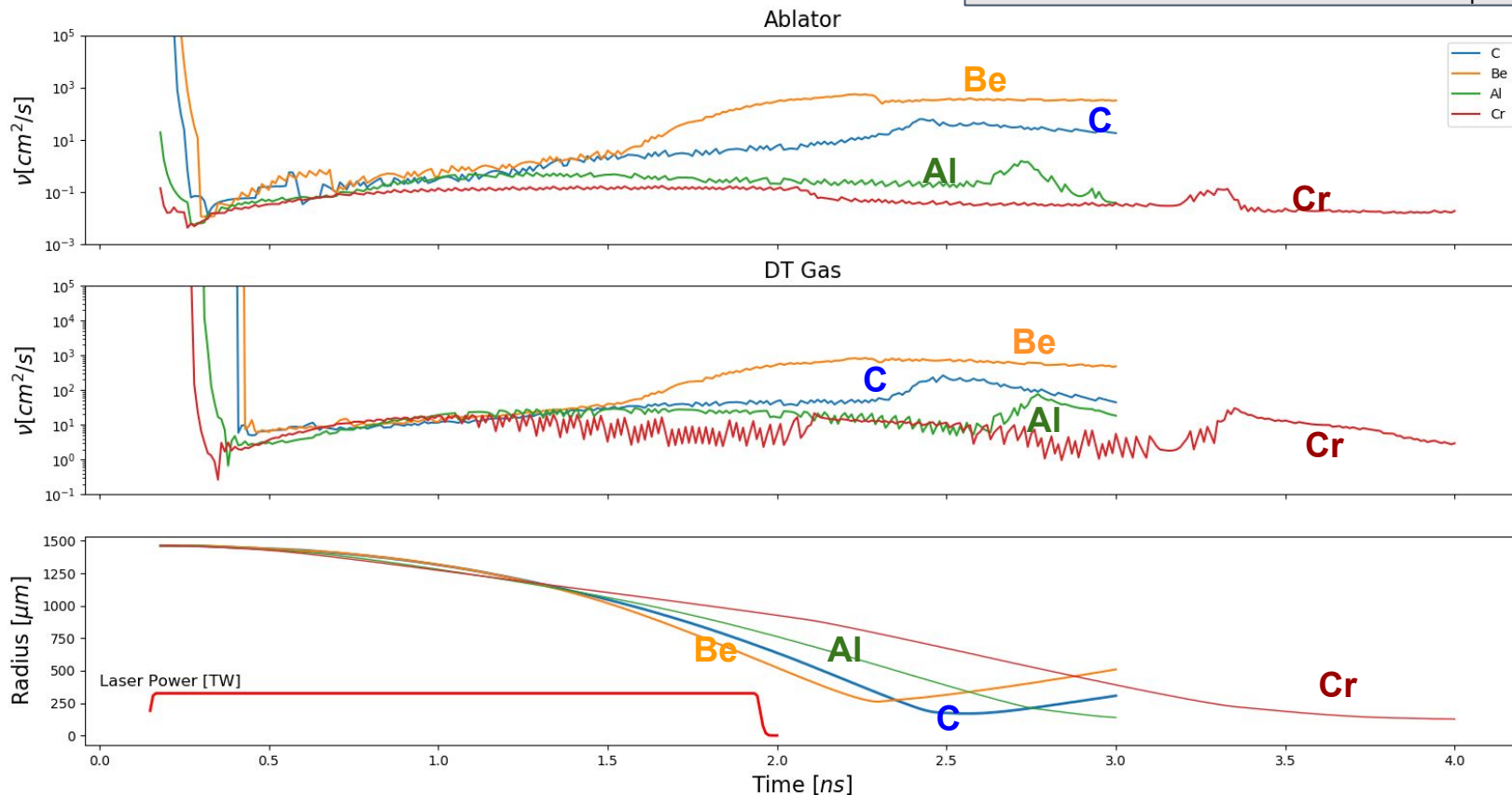
$$\begin{aligned} \eta^*(\Gamma) &= \frac{\eta}{mna^2\omega_p} \\ &= \frac{a}{\Gamma^{5/2} \ln\left(1 + \frac{b}{\Gamma^{3/2}}\right)} \frac{1 + a_1\Gamma + a_2\Gamma^2 + a_3\Gamma^3}{1 + b_1\Gamma + b_2\Gamma^2 + b_3\Gamma^3 + b_4\Gamma^4} \end{aligned}$$

J. Daligault et al. Physical Review E90, 033105 (2014)



Kinematic Viscosity along Material Interface for Square Wave Laser

$$\text{Kinematic Viscosity: } \nu = \eta^* a^2 \omega_p$$



Instability Growth Rate for Square Wave Pulse

Amplitude of Instability

$$a_k(t) = a_k(0)e^{\gamma(k)t}$$

Instability Growth Rate

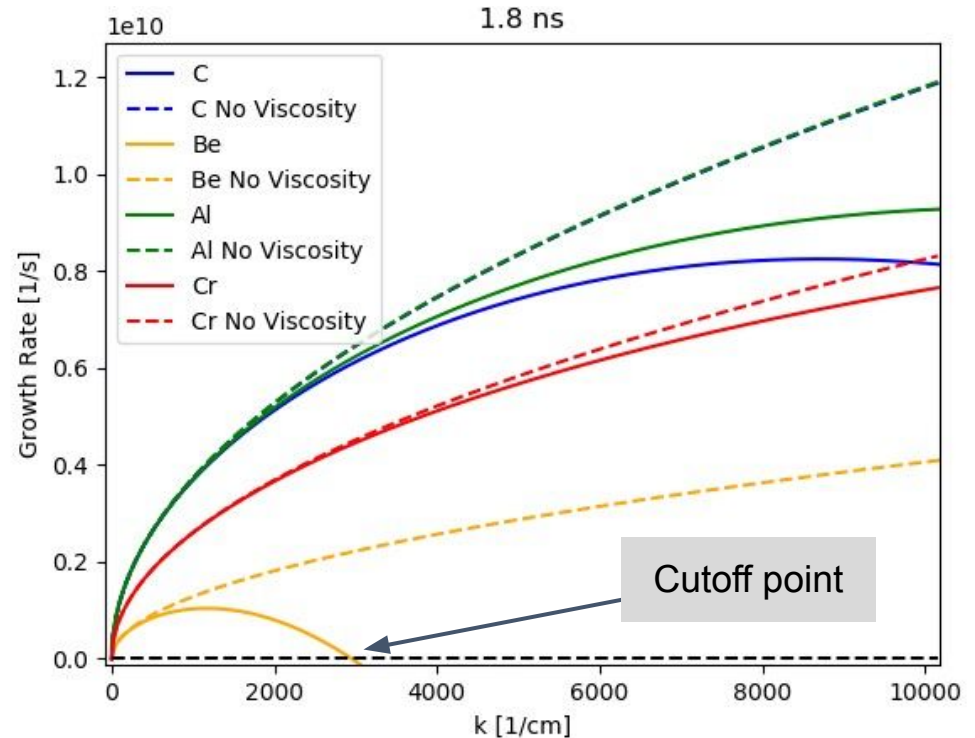
$$\gamma_I = \sqrt{Ak\ddot{R}/\eta + \nu^2 k^4} - (\nu + D_{12})k^2,$$

ν = kinematic viscosity

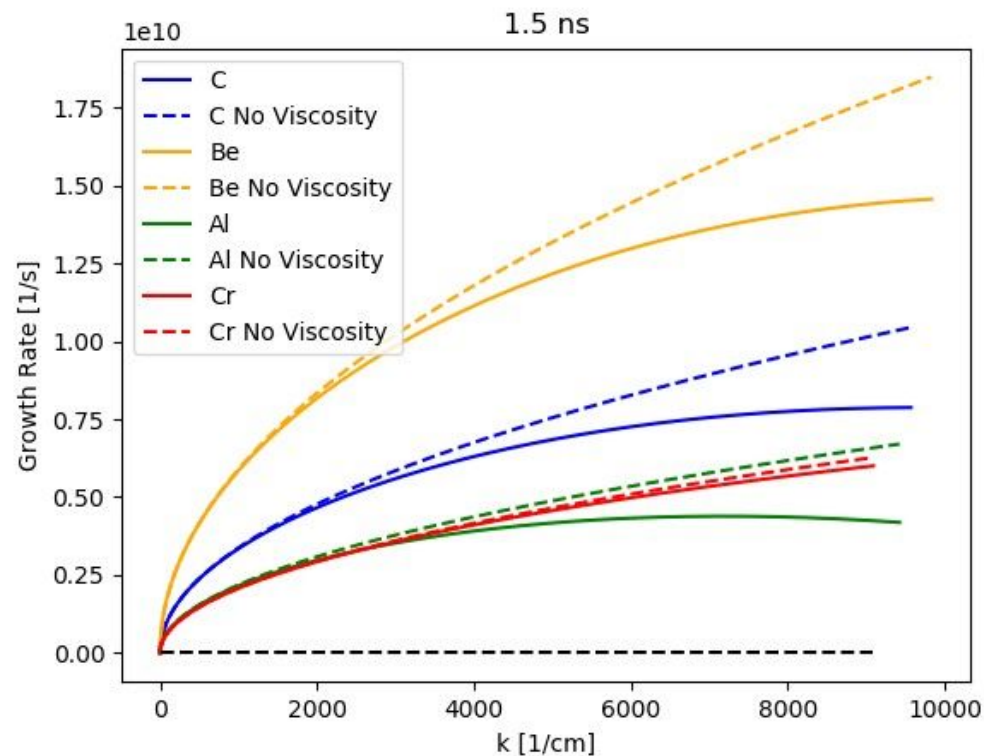
A = density ratio of DT Gas to Ablator

k = wave number

\ddot{R} = acceleration at material interface

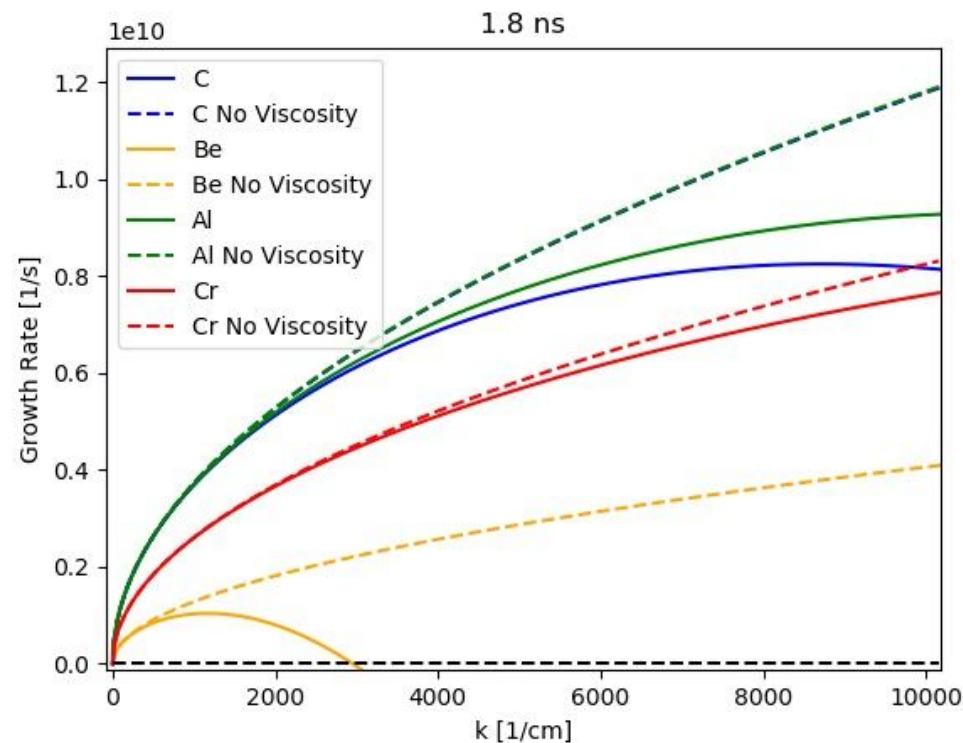


Instability Growth Rate for Square Wave Pulse in DT Gas



1.5 ns						
	v_{Shell} cm ² /s	v_{Gas} cm ² /s	A	R_{um}	\ddot{R} cm/s ²	Z Shell
C	1.718	28.17	0.282	1040	-4.407	3.85
Be	3.842	40.59	0.355	1020	-0.093	2.63
Al	0.456	28.48	0.275	1015	-2.563	6.96
Cr	0.124	3.28	0.296	1098	-4.602	12.83

Instability Growth Rate for Square Wave Pulse in DT Gas



1.8 ns						
	v Shell cm ² /s	v Gas cm ² /s	A	R um	\ddot{R} cm/s ²	Z Shell
C	2.88	36.38	0.246	789	-5.191	3.66
Be	94.26	253.6	0.074	699	-2.636	2.195
Al	0.287	25.59	0.329	870	-3.960	7.922
Cr	0.144	6.40	0.295	980	-7.324	11.37

Conclusions

One-Component Materials

- Adding pickets to the pulse shape did not affect the viscosity substantially.
- While Be seems to be most effective in dampening instabilities while Cr is the least effective.

MD-Simulation of TCP

- LAMMPS TCP input deck was successfully verified against OCP simulation.
- Successfully calculated the viscosity of a CH TCP for a range of Γ values.

Future Work

- Submitted Abstracts to the Division of Plasma Physics (DPP) Annual Meeting and will present work there
- Continue working with Brett Scheiner on two-component plasmas.